High-Order Methods for Nanophotonics

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Summary

Argonne researchers have recently developed high-order methods in electromagnetics that demonstrate exponentially accurate computational results. Further development of the methods and successful extension to the application in nanophotonic waveguides and photonic crystals will significantly increase the importance of higher-order methods and their use by the optics community.

In the study of light interacting with a metallic nanoscale object, a particular computational issue is that the problem includes sharp discontinuities in the dielectric function along the surface of the metallic object. In such cases, standard lower-order methods require considerable computational work in order to achieve a certain expected accuracy. The drawback stems from the slow rate of convergence of the methods for discontinuous problems or problems whose solutions have less regularity in smoothness.

Argonne researchers have been developing and analyzing efficient and accurate high-order numerical methods for the study of electromagnetic wave propagations for nanophotonic and photonic crystal waveguide problems. Three high-order numerical techniques have been developed for those problems: pseudo-spectral Fourier time-domain method combined with postprocessing techniques, spectral-element methods (SEM), and discontinuous Galerkin spectral element methods (DG-SEM).

We applied the standard pseudo-spectral Fourier time-domain method (PSTD), combined with postprocessing techniques such as Gegenbauer and Pade´ reconstruction, to nanophotonic problems. Since pseudo-spectral methods are global methods, numerical artifacts such as high oscillations (Gibb's phenomena) deteriorate the approximate solutions because of the nonsmoothness between materials. Careful numerical analysis, however, reveals that the PSTD method retains accurate phase information despite the oscillatory nature of standard Fourier reconstructions. Gegenbauer postprocessing, applied at a final time step to PSTD solutions, successfully enhances their accuracy and provides an accurate reconstruction.

Figure 1 shows the original (top left) and Gegenbauer reconstructed (top right) results based on 512 x 512 PSTD data. The Gegenbauer reconstruction eliminates the nonphysical oscillations of the original PSTD calculation. The reconstructed results agree well with the finer resolution finite difference time domain (bottom) results away from the metal boundary. Moreover,

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near the material interface, Gegenbauer-postprocessed results successfully capture a more physically reasonable profile.

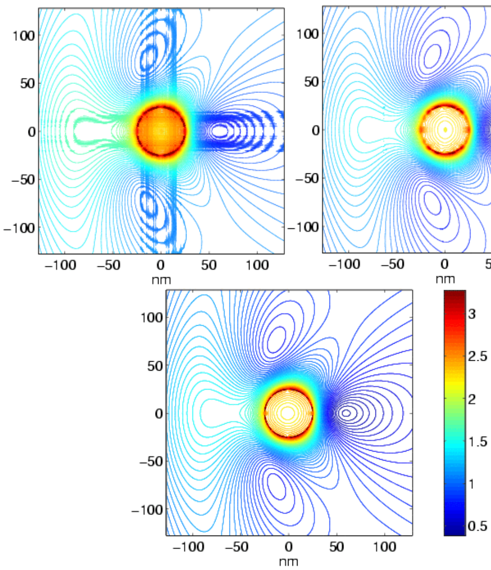

Figure 1. Incident plane-wave field response computed with PSTD (top left), PSTD + Gegenbauer reconstruction (top right), and finite differences (bottom). Resolution is 512 x 512 (top) and 2560 x 2560 (bottom).

We have also demonstrated that DG-SEM and SEM are very effective for simulating propagation of electromagnetic waves in free space and for computing Maxwell's eigenvalue problems in one and two dimensions. We split the domain into subdomains in a way that the dielectric function in each subdomain is smooth. This approach reformulates the problem as continuous in each subdomain, and we use high-order spectral bases within each subdomain. These methods retain many of the advantages of the PSTD method (principally, minimal numerical dispersion), while avoiding the Gibb's phenomenon entirely. Contrary to conventional low-order methods that give generally second-order or at most third-order convergence, the spectral-element method can dramatically reduce the computational cost in two- and three-dimensional problems with high accuracy.

We also have developed discontinuous Galerkin spectral element codes for electromagnetics problems incorporated into Argonne's spectral-element code Nek5000, which is recognized for its algorithm quality and scalability. With these codes, we are carrying out time-domain simulations of propagating plane waves impinging on a nanocylinder. A criticial development for the simulation of practical problems has been the incorporation of perfectly-matched-layer boundary conditions that admit reflectionless outgoing waves.

In the coming year, we plan to extend this work to two- and three-dimensional studies of nanophotonic waveguides for various structures and to periodically structured photonic crystals.

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